Predictive Science Academic Alliance Program (PSAAP)

The slides that follow were presented at the PSAAP Bidder's Meeting May 16-17, 2006 and represent the ASC Trilab authors and interests as presented in the associated White Paper for this subject area.

Equation of State and Constitutive Properties

John Aidun (SNL)

Christian Mailhiot (LLNL)

Tommy Sewell (LANL)

Predictive Science Academic Alliance Program

Bidders' Meeting

Dallas, TX

May 17, 2006

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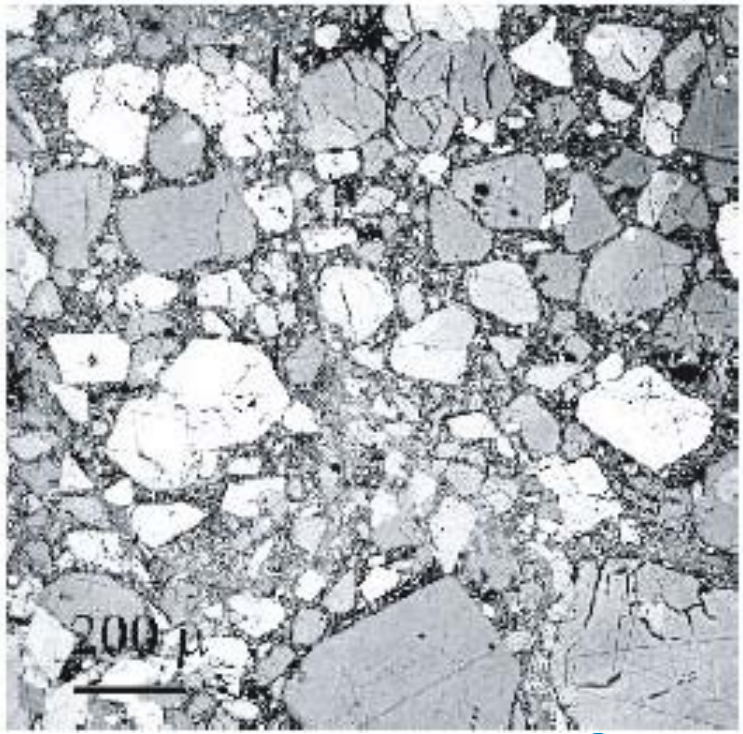
Equation of State and Constitutive Properties

- Accurate, physics-based constitutive models and fundamental properties are absolutely essential to development of a truly predictive scientific simulation capability.
- Multiscale, strongly heterogeneous materials under a wide variety of thermodynamic and dynamic loading conditions
- Pristine, aged, and damaged states
- Requirement: quantified accuracy & reliability



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Thermodynamic Properties

- EOS establishes fundamental relationships among thermodynamic variables, provides closure of hydrodynamic equations
- Typically well-defined on atomic scales
- Often directly accessible, in principle, to atomistic simulation *(with caveats)*
- EOS, phase boundaries, re-solidification, transport and mechanical properties
- Wide range of thermodynamic states of interest
- Required as input to mesoscopic and continuum constitutive models

Engineering Constitutive Properties & Models

- Typically governed by phenomena occurring across multiple length scales
- Often dominated by collective behavior of defects, material interfaces, and evolution of material microstructure
- Spatial resolution of practical applications necessitates use of sub-grid models
- Usually phenomenological in nature

Predictive HE Detonation Products EOS

Goal: Utilize ab initio quantum chemistry to develop accurate HE detonation products EOS.

People: M. Sam Shaw, C.J. Tymczak (LANL, T-14)

MondoSCF is ab initio linear-scaling DFT quantum chemisty code developed by LANL ASC (Challacombe, et al.) that includes exact exchange (e.g., PBE0 6-31G).**

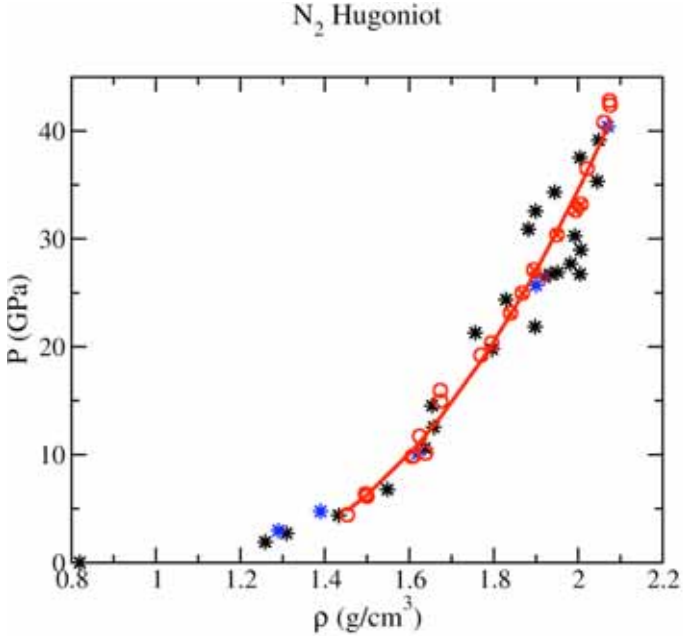
Perform 20-100 calculations for each P,T point where configurations are sampled from classical Monte Carlo simulations (100K) with potentials matched to ab initio functions.

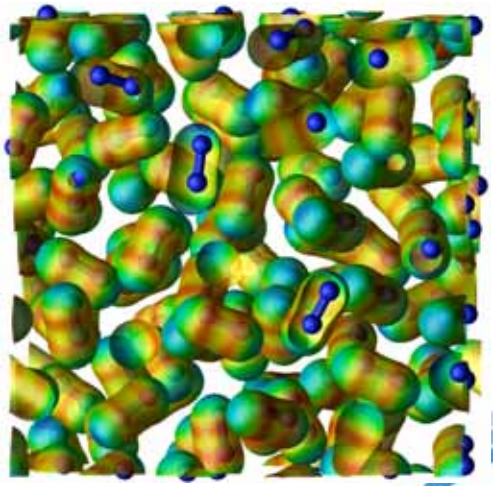
Experimental data (*) have error bars that extend to central curve. Calculated points (O) have error bars of similar size to the symbols.

Corrected sampling of configurations generated from model potentials, correction of potentials

Basis set and sample size convergence

Development and bounds of cross-potentials





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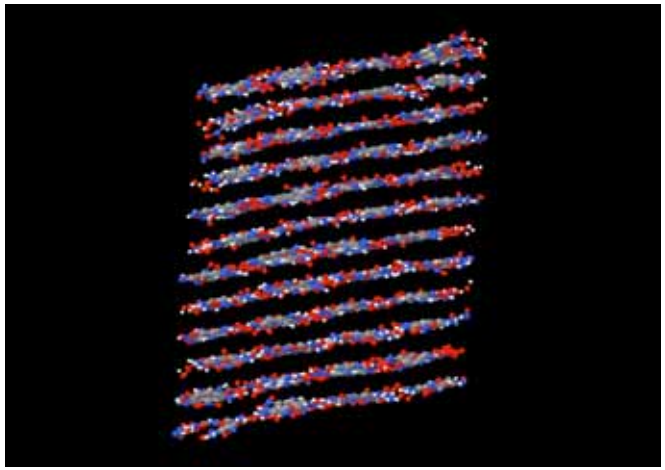
HMX Crystal Bulk Modulus

K (GPa), K'	Comment	Authors	Publication/year
13.5, 9.3 0-7.5 Gpa	Isotherm fit: U_s-U_p EOS	Olinger et al.	CEA Conference proceeding, 1978
12.4*, 10.4 0-27 GPa	Isotherm fit: 3rd-order Birch-Murnaghan EOS	Yoo & Cynn	J. Chem. Phys., 1999
14±3.5, 7.5 ± 1.9	Re-analysis of experimental data	Menikoff & Sewell	High Press. Res., 2001
14.53, 9.57 (*P2$_1$/c*) **16.86**, 9.50 (*P2$_1$/n*) 0-7.5 GPa	Isotherm fit: Murnaghan EOS (Atomistic simulation)	Sorescu et al.	J. Phys. Chem., 1999
15.1 (C_{ij}) **15.5-16.3**, 11.0-12.1 (EOS, 0-10 Gpa)	Isotherm fits and **C_{ij}** (Atomistic simulation)	Sewell et al.	J. Chem. Phys., 2003
21.0 ± 1.0, 7.45 ± 0.95 0-5 GPa	Isotherm fit: 3rd-order Birch-Murnaghan EOS	Gump & Peiris	J. Appl. Phys., 2005
9.9 (from isentropic C_{ij})	Brillouin zone scattering	Stevens & Eckhardt	J. Chem. Phys., 2005

Prediction of TATB Elastic Tensor

Snapshot from simulation of TATB crystal with 10% porosity at T=295 K, P=1 atm.



Objective: Calculate isothermal elastic tensor for TATB crystal as function of temperature, pressure, and crystal purity

People: Tommy Sewell, Dmitry Bedrov (Utah), Rick Gee (LLNL)

- Force field of Gee et al. (LLNL, '04) implemented in Lucretius MD code
  - Minor change to original: ignore intramolecular non-bonded terms
- Computed structure, elastic tensor for T= 195 - 395 K, P=0-3 GPa
  - 4x4x6 super cell (192 molecules)
  - Results are still preliminary
  - Considering effect of randomly distributed porosity (0, 5, 10%)

Case	K_{Reuss}	K_{Voigt}	G_{Ruess}	G_{Voigt}
Pure	10.2	25.7	2.8	14.7
10% porosity	6.1	15.9	1.4	9.3

Preliminary predictions of isotropic moduli, obtained from the full elastic tensor at T=295 K, P=1 atm. Units are Gpa.
Reuss ⇒uniform stress, Voigt ⇒uniform strain

Case	C_{11}	C_{22}	C_{33}
Pure	82.6	73.8	11.6
10% porosity	51.6	47.4	7.2

Preliminary predictions of C_{11}, C_{22}, C_{33} for T=295 K, P=1 atm. Units are Gpa.

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Phase Transitions, Melt, and Solidification

Major effects on material response

material strength, microstructure, chemistry

Pure elements, alloys, molecular compounds of interest

Phase boundaries, mechanisms and kinetics of transformation

Physics of phase transitions at interfaces

Frustration and metastability

Atomic- through continuum-scale descriptions

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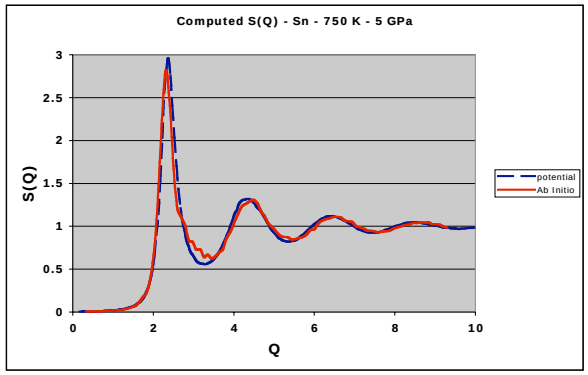
MD simulation of pressure-driven solidification provide kinetic data

S. Foiles, J-P Davis - SNL



Novel interatomic potential for Sn developed that reproduces DFT based liquid structure at high pressures

- Simulations provide the microscopic kinetic coefficient
  - Interface velocity as a function of under-cooling / over-pressurization
- Simulations provide the solid-liquid interfacial free energy
  - Key parameter in rate of homogeneous nucleation

Predicted points on liquidus

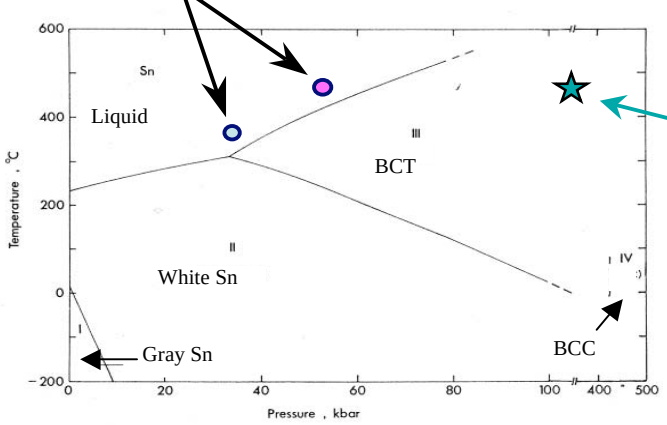
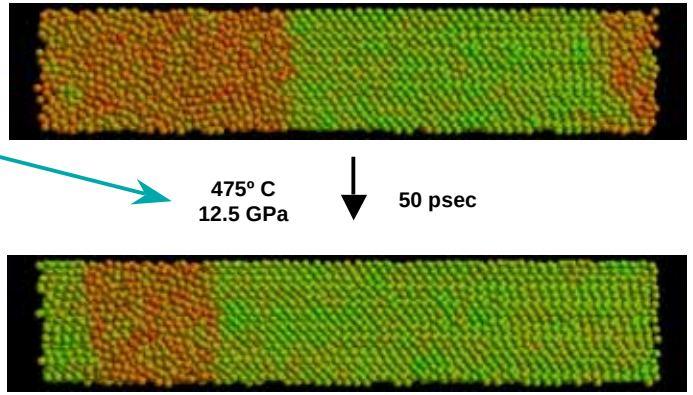


Fig. 2.17. Phase diagram of Sn.



Freezing is simulated directly with MD (Red-orange atoms are liquid)

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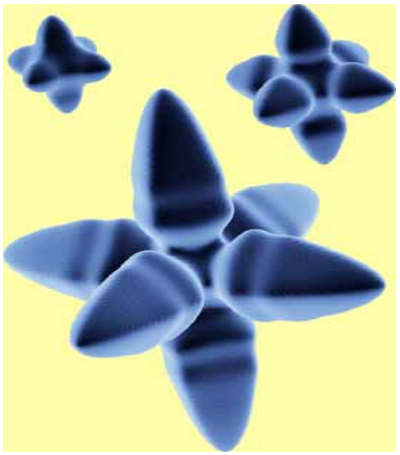
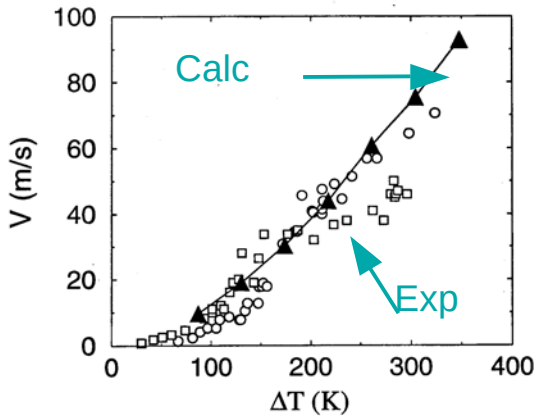
Mesoscale modeling of solidification connects microscopic parameters to the overall freezing rate

J. J. Hoyt - SNL



Dendrite Tip velocity



- Demonstrated connecting atomistic simulations to mesoscale for conventional solidification
- Mesoscale models will provide the overall freezing rate required to correlate measurements with liquid-solid transition
- Approaches
  - Nucleation and growth models
    - Volume fraction as a function of time/temperature/pressure
  - Phase Field model of solidification

Parameter free prediction of dendrite growth velocity in highly under-cooled Ni. (Bragard et al., 2001)

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Optical, Electrical, and Transport Properties

- Often measured experimentally, thus the ability to predict these quantities from first principles and relate them to thermodynamic state is of great importance
- Examples: optical properties of shocked materials, electrical conductivity of materials at high temperature

Constitutive Model Formulations

- Need for material properties well beyond linear regime (e.g., plasticity or failure)
- Single- as well as multi-material treatments
- Strongly-coupled physics
- Strongly-driven conditions
- Robust, efficient algorithms
- Extensive verification and validation

PBX-9501 Detonation

Ralph Menikoff (LANL)

Model I (r): Menikoff
- Solid: Birch Murnaghan (Sewell, Menikoff, 2004)), C_v = Goddard QC
- Gas: Sesame (Shaw, 2004)
- Reaction: Arrhenius (Henson, 2002)
- Does not do initiation (Pop plot)

Model II (b): Stewart, Lambert
- Solid: Wide-Ranging EOS (Davis, 2004): $C_v = k\ S$
- Gas: WR EOS (Davis, 2004)
- Reaction: Single-step P^n
- Also fits Pop plot data

Model III (g): Tarver I&G
- Solid: JWL (Tarver), $C_v = C$
- Gas: JWL (Tarver)
- Reaction: time constant and two step P^n
- Also fits Pop plot data

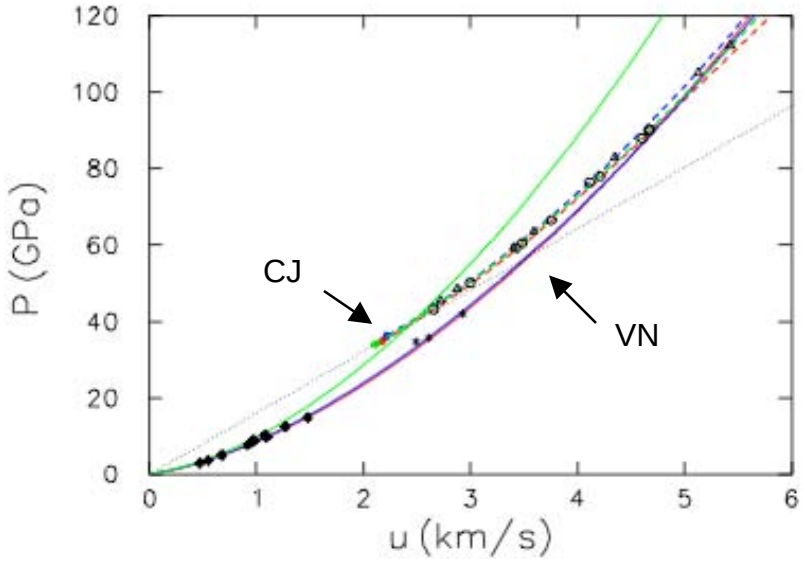

Table 1: Von Neumann spike and CJ states for detonation wave in PBX 9501 based on the model equations of state.

	Model I	Model II	Model III	
ρ_0	1.833	1.844	1.835	g/cm^3
D	8.77	8.86	8.80	km/s
VN spike				
P	56.9	59.0	39.6	GPa
ρ	3.07	3.11	2.54	g/cm^3
u	3.55	3.61	2.45	km/s
T	2581.	1801.	1550.	K
CJ state				
P	34.9	36.3	34.0	GPa
ρ	2.43	2.46	2.41	g/cm^3
u	2.17	2.22	2.11	km/s
T	3000.	3500.	5372.	K

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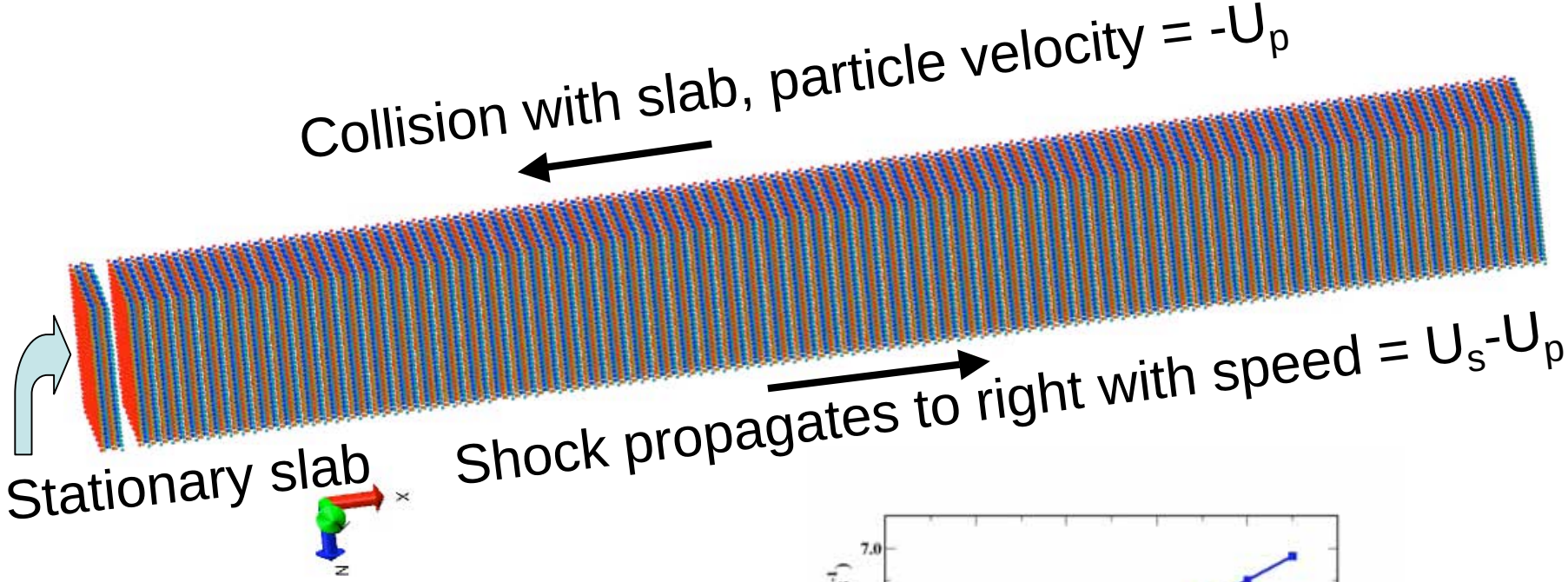
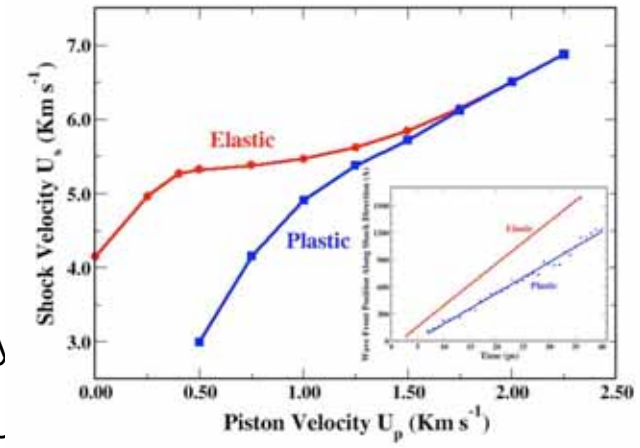
HMX Shock Compression Studies

Jaramillo (LANL), Strachan (Purdue), Sewell (LANL)

- **245760 Molecules = 6881280 Atoms (C-H bonds fixed)**
- **System Size: 184.27 x 19.27 x 19.47 nm**

α–HMX – 249856 Molecules – Shock Direction <100> – Up = 0.75 Km/s – Jaramillo, Strachan and Sewell – LANL T–14





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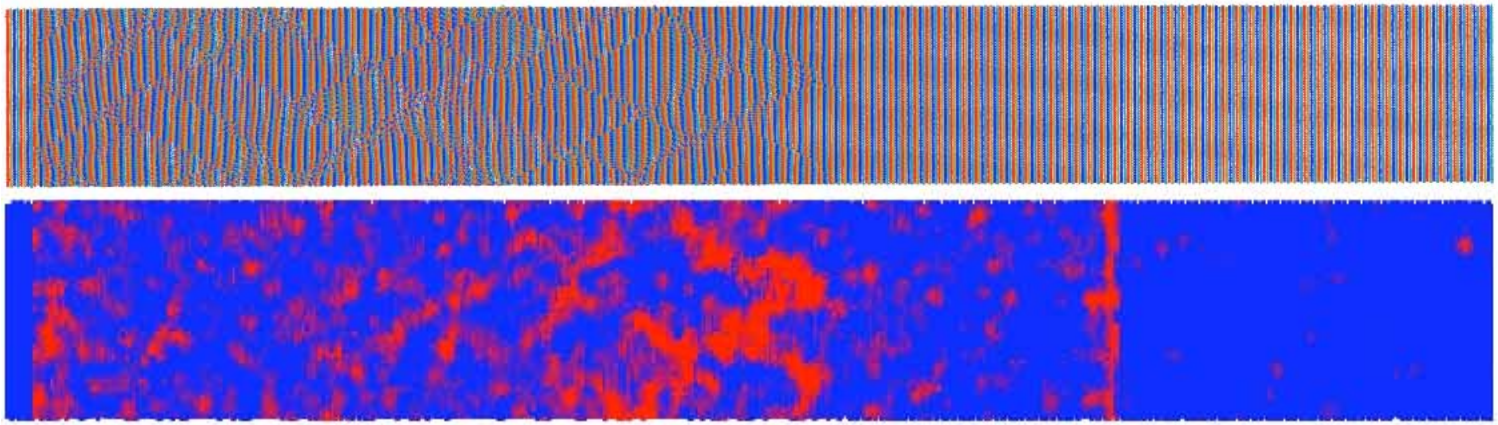
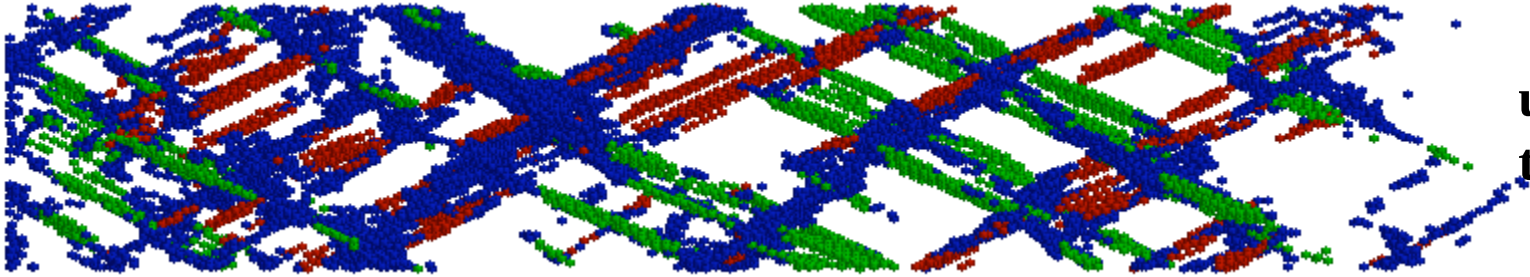
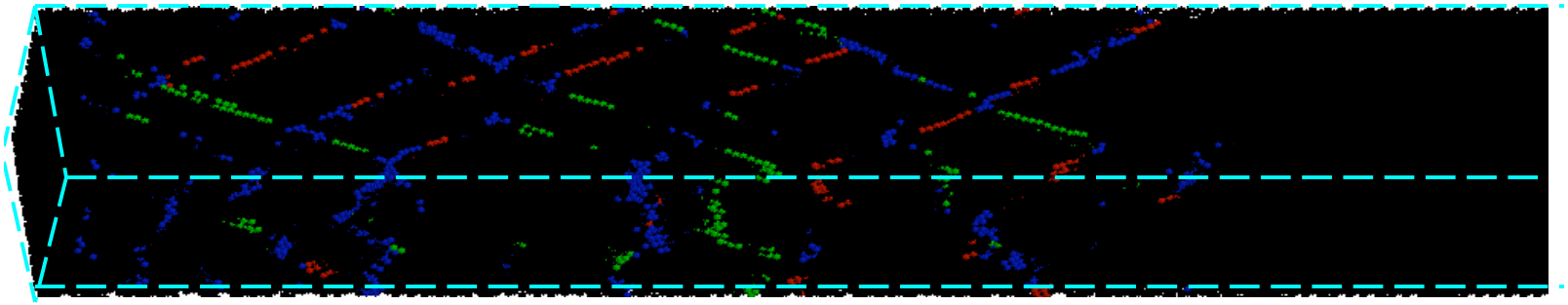
HMX Local Temperature, Plastic Activity
Jaramillo, Strachan, Sewell



u_p=0.75 km/s
t=28 ps



u_p=0.75 km/s
t=35 ps



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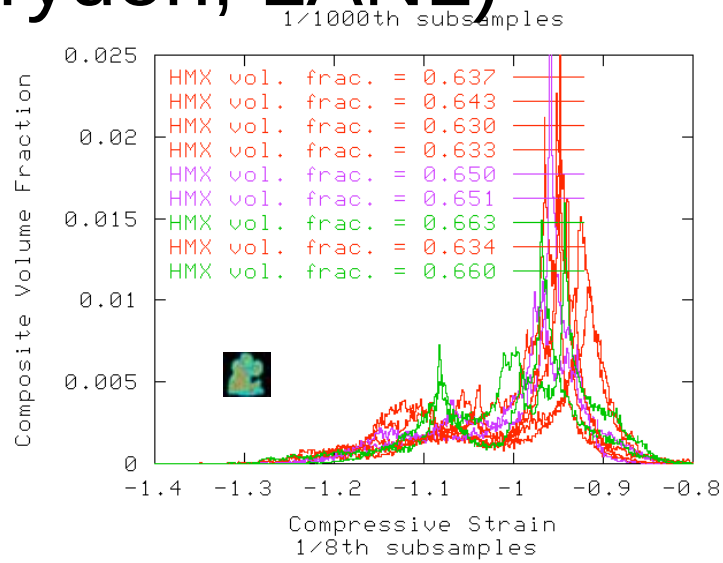
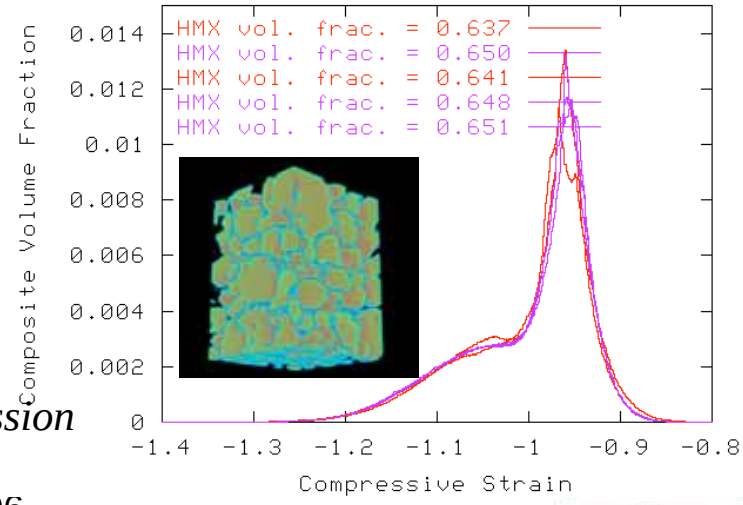
Polycrystal and Multi-Material Elasticity and Plasticity

- Even anisotropic single-crystal elasticity is difficult to obtain in practice
- Sensitive stress, temperature, and strain-rate dependencies; also, damage and defects
- Polycrystal response requires homogenization over an appropriate representative volume element (RVE)
- Metals, organics, piezo- and ferro-electrics, random and ordered composites
- Complicated time histories

PBX Constitutive Modeling
(Bardenhagen and Brydon, LANL)

- Continuum constitutive theory predicts Plastic-Bonded Explosive (PBX) bulk response given microscale strain statistics.
- Simulations used to generate strain statistics
  - PBX Microstructures obtained from microtomography
- *Smallest sample size ( ) gives accurate bulk properties* (moduli)
- Statistical Representative Volume Element (RVE) ~80x bigger.





Strain Statistics

To appear in *Shock Compression of Condensed Matter - 2005*

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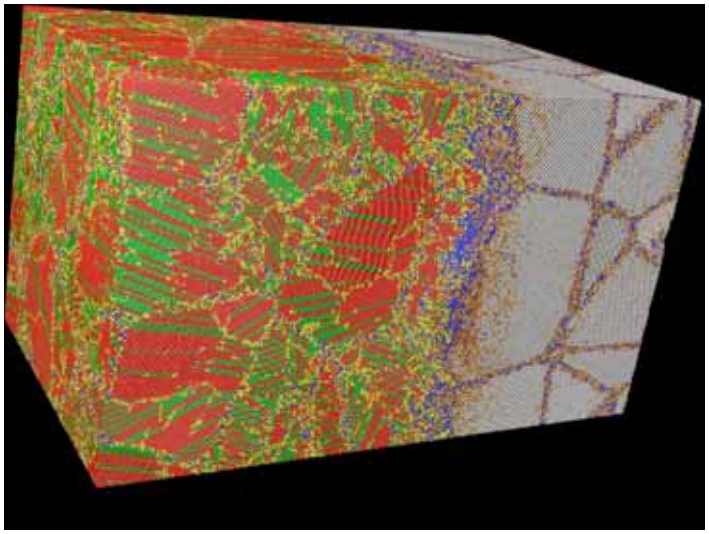
SPaSM: Massive Parallel MD to Characterize Shock Response

Shock-induced transformation mechanism in Fe single crystals predicted by large-scale molecular-dynamics simulations*

NEMD results confirmed experimentally** by ultrafast (nanosecond) X-ray diffraction (shocks and high intensity X-rays produced by high energy laser systems OMEGA/Janus/Vulcan)

*K. Kadau,T. C. Germann, P.S. Lomdahl, B. L. Holian, *Science* **296** 1681 (2002).

** D.H. Kalantar et al., *Phys. Rev. Lett.* **95**, 075502 (2005)

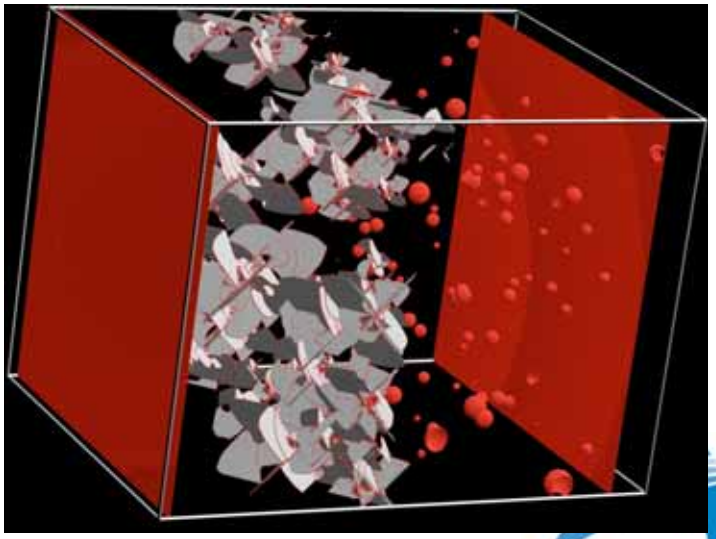


EAM poly Fe 30 M atoms 256-CPU of Linux Cluster Pink Bcc (gray), 10c (blue) 11c (yellow), hcp (red) fcc (green)***,****

***K. Kadau,T. C. Germann, P.S. Lomdahl, B. L. Holian, R. Albers, to be submitted to *Phys. Rev. Lett.* (2006).

**** B. Yaakobi et al., *Phys. Rev. Lett.* **95**, 075501 (2005)

The effect of an aging-induced small density (~1%) of voids (vacancy clusters) in a metal on the resulting shock Hugoniot, temperature, plastic response, etc. upon loading as the voids partially collapse.



EAM Cu, U_p = 200 m/s, 17 ps

Centrosymmetry parameter to show only hcp (grey) and defect (red) atoms

271 nm × 271 nm × 343 nm, with 0.41% porosity ⇨ **2,131,656,770 atoms**

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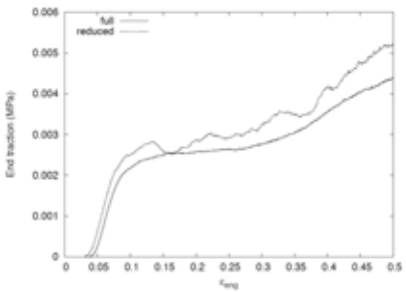
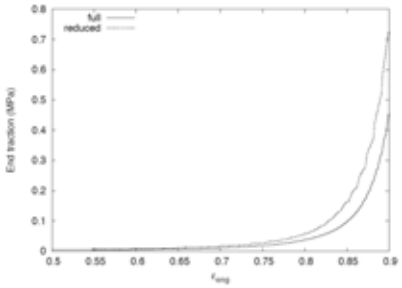
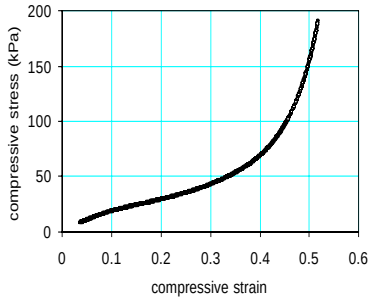
Compression of Real Foam Microstructures (Bardenhagen and Brydon, LANL)

- Derivatives of basic Particle-In-Cell (PIC) Method
- Governing equations solved on grid.
- Particles used to advect solution variables.
- No mesh distortion, large material deformations
- Complex geometries easily discretized; importing data from X-ray tomography
- Material Point Method
- Wide variety of materials models readily incorporated
- Robust contact algorithm ((*Bardenhagen et. al., Comput. Model. Eng. & Sci., 2 (2001), 509*)
- Improved interpolation method: GIMP (Bardenhagen, in press)
- Generate PDF's and RVE's for homogenization models
- Incorporate fundamental physics models as available

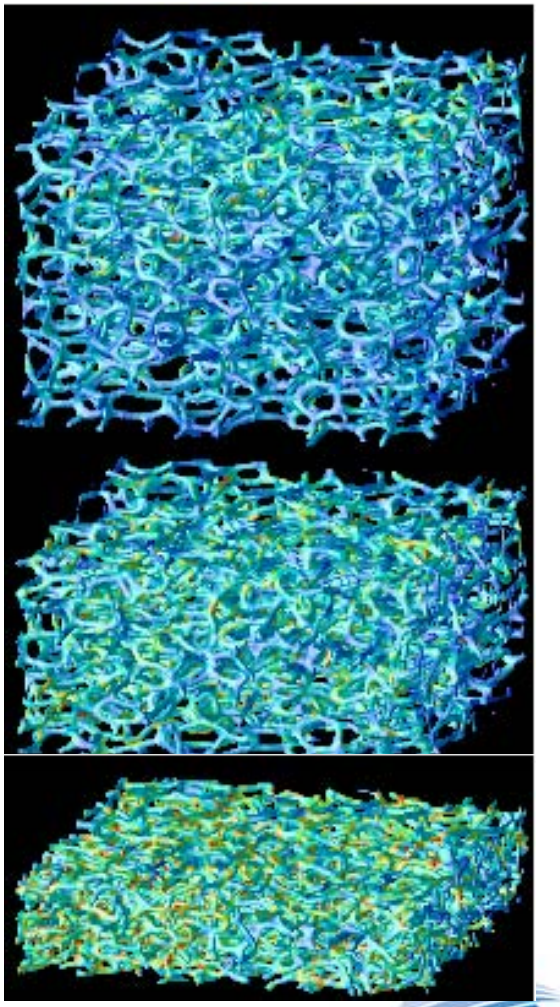




Calculated results of foam compression for shown sample size and 1/8 sized sample



Typical results for foam compression curve



Stress field of urethane foam at 10, 50 and 90% compression

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Interfacial Phenomena

- Material interfaces often dominate constitutive behavior
- Many materials of interest have huge interfacial areas
- Interfaces can be sharp or diffuse, can serve to localize stress, and can affect material stability/compatibility
- Both physical and chemical processes at interfaces are of interest
- Need for simulation/theory advances on all scales

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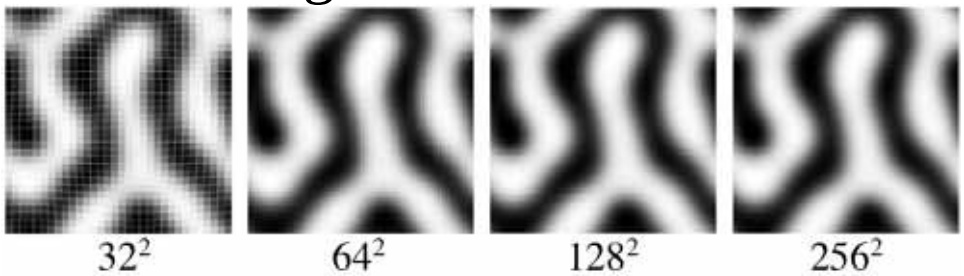
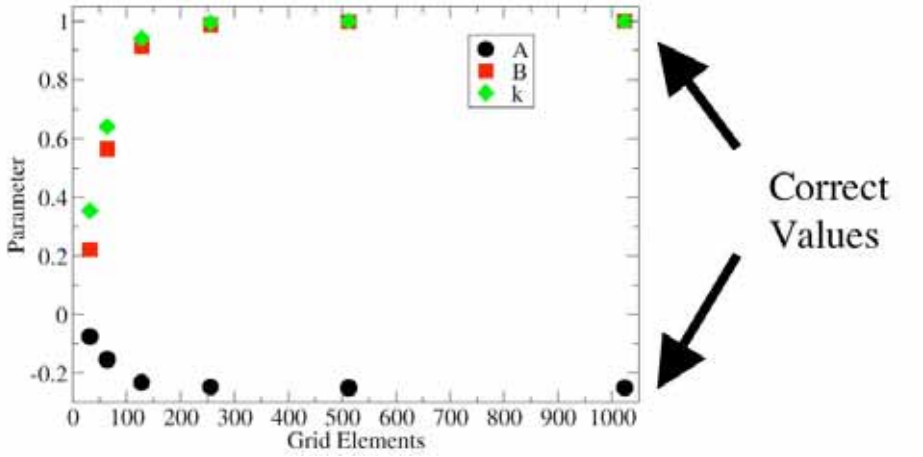
Inverse Time-Dependent Ginzburg-Landau on Polymer Blends

Goal: Fit the TDGL Equation of Motion

$$\partial_t \psi(R,t) = \Lambda \nabla^2 (A\psi + B\psi^3 - \kappa \nabla^2 \psi)$$

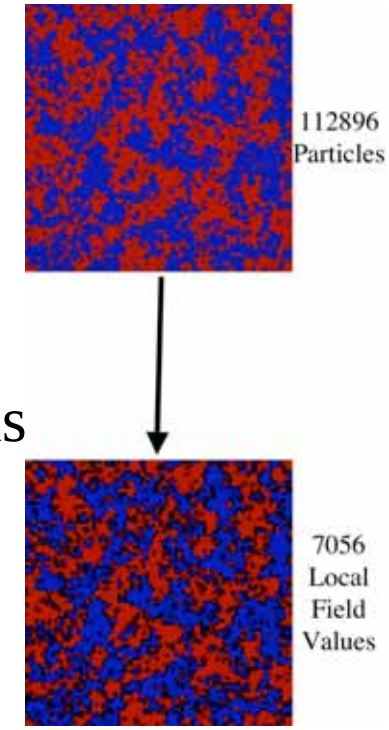
Inverting TDGL Simulations

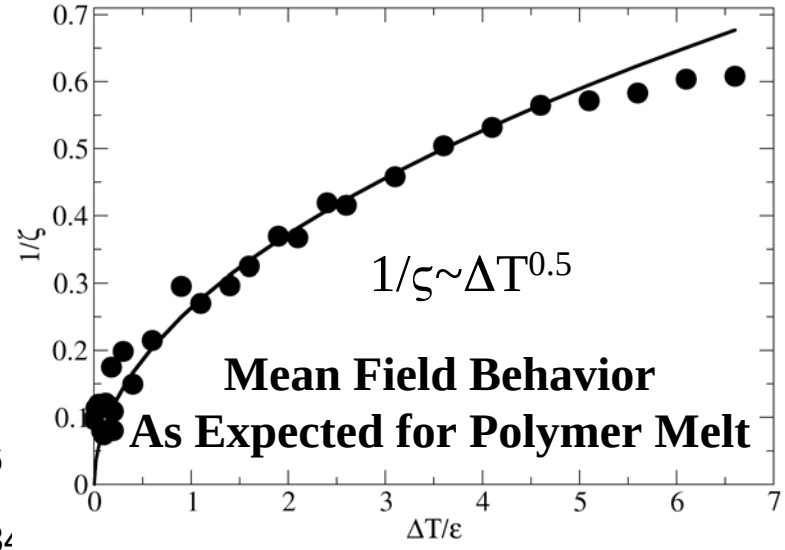




Correct Values

Inverting MC Simulations





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Homogenized Treatment of Damage, Cracking, and Failure

- Material heterogeneity, localization and damage are inherently multi-scale
- Generally required to treat sub-scale phenomena within engineering-scale simulations
- Need physically-based, quantifiable and measurable connections among atomistic, mesoscopic, and anisotropic continuum-scale simulation models and methods